Researchers examine behavior of amorphous materials under high strain

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Disordered solids such as plastics, window glass, and amorphous metals possess many useful applications. Industrial processing of these materials commonly involves plastic deformation. The physical processes controlling the onset of yield, where a material changes its shape permanently under external deformation, are not yet understood for amorphous solids. The problem is key to understanding how a solid can fail. In findings published in *Nature Communications*, a research team from LANL, Harvard University, and the University of Illinois-Urbana Champaign have found strong evidence that the point at which a disordered or amorphous solid begins to yield and flow under an applied stress exhibits features similar to those found in the study of chaos, as well as well as the phase transition from one state of matter to another.

Significance of the research

The transition to flowing behavior in systems as diverse as earthquakes, charge density waves, and disordered magnets is accompanied by the occurrence of avalanches of increasing sizes obeying power-law statistics, a signature of critical behavior. The new publication shows that in amorphous solids, at the same critical strain amplitude where irreversibility occurs, the system undergoes a non-equilibrium phase transition involving avalanches of diverging sizes.

This phenomenon offers a new way to define the yield point in an amorphous solid, and therefore the ability to monitor the onset of plastic deformation and thus mechanical properties of materials ranging from everyday plastics to bulk metallic glasses where strength, hardness and toughness are important. This is particularly relevant at the design stage where it is important to assess performance under strong impact. If these ideas extend to a broader class of systems, it would allow researchers to produce new predictive tools to examine the fluctuations or avalanches in a system to determine whether it is close to some kind of critical transition or failure, giving time to prepare for or mitigate the failure process.

Research achievements

The team performed large-scale molecular dynamics and mean-field theory simulations of systems of 1,024, 4,096 and 16,384 particles interacting in two dimensions. The researchers found that under periodic shearing, atoms rearrange themselves in avalanches or sudden bursts of activity. Below a critical strain, the system organizes to a state where the avalanches are exactly repeated and the atoms return to their previous positions at the end of each cycle. As the strain increases, there is a critical strain point above which the avalanches do not exactly repeat and the atoms no longer return to the same positions at the end of the cycle.

The authors had already established that the transition point is accompanied by cycles of ever increasing periodicity during which particles change their mechanical equilibrium positions but follow the same trajectories for consecutive cycles. Above a critical strain amplitude, the system does not settle into a limit cycle. The motion transitions to chaotic behavior, very reminiscent of systems undergoing nonlinear dynamics with initial close-by positions diverging exponentially with time and losing all memory of the initial state. This transition point coincides with a divergence in the time scale. This behavior is consistent with what is called criticality, which occurs for certain phase transitions where specific quantities at the transition can have universal features independent of the details or nature of the system. The result implies that the system out of equilibrium undergoes a nonequilibrium phase transition where energy is being pumped into it and dissipated.

The research team

The researchers include Ido Regev, Charles Reichhardt and Turab Lookman of LANL's Physics of Condensed Matter and Complex Systems group and the Center for Nonlinear Studies (CNLS) and John Weber and Karin A. Dahmen of the University of Illinois at Urbana Champaign. Regev is now a postdoctoral fellow at Harvard University.
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